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High-Performance Computing & Air Turbulence/Pollution Studies

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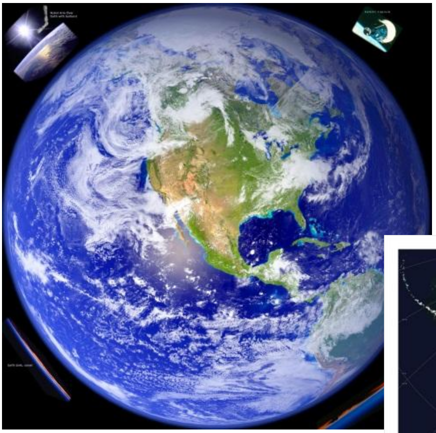
Tutorial Outline

- Why high-performance computing?
- Methodology
- LESChem results
  - Ventilation & pollutant removal
  - Buoyancy & temperature stratification
  - Chemically reactive pollutants
- Conclusion
- Upcoming Work

Why high-performance computing? [1/2]

- The atmospheric boundary layer (ABL) is too large to measure
- Broad spectrum of fluid motions
- The variables are uncontrollable

Global scale



Continental scale

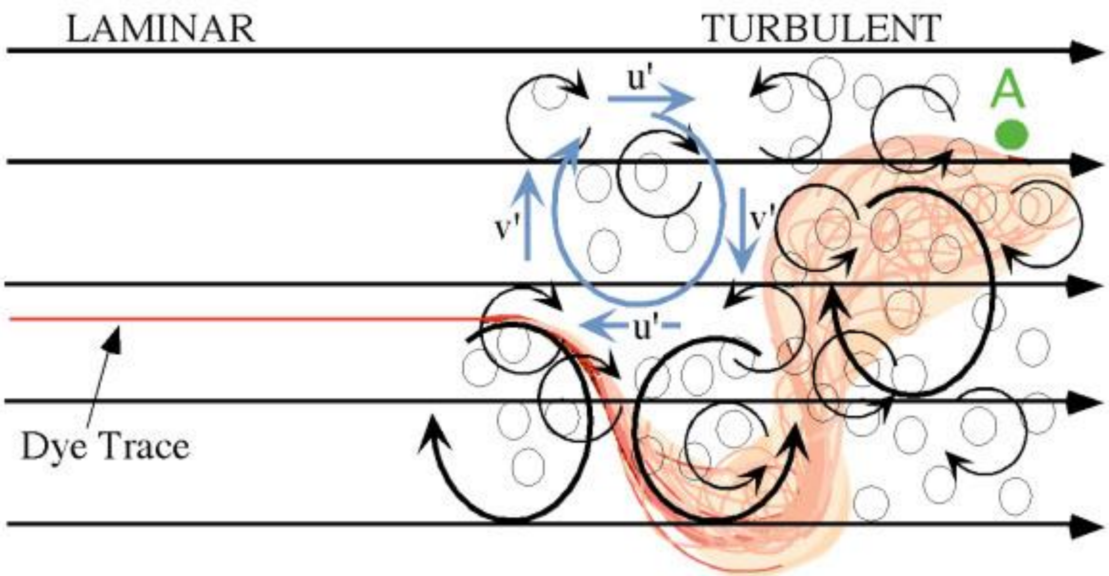
Natural terrain

City-scale

Street level

Why high-performance computing? [2/2]

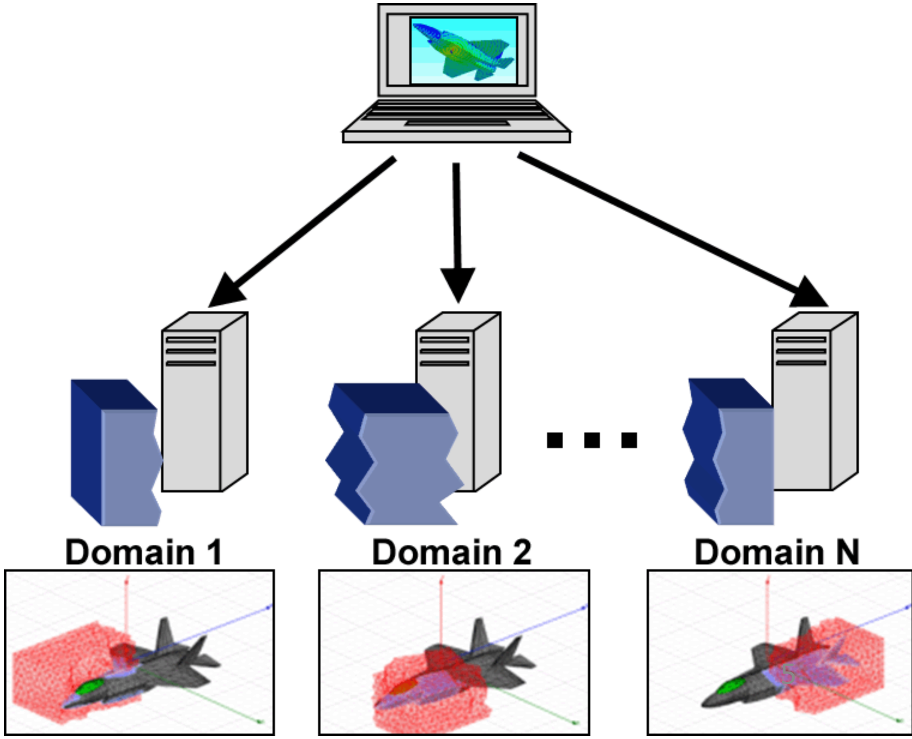
- Turbulence
  - Multi-scale transient motions
- Buoyancy & temperature stratification
  - Instability and chaotic motions
- Coupled physics & chemistry
  - Nonlinear solution



Methodology

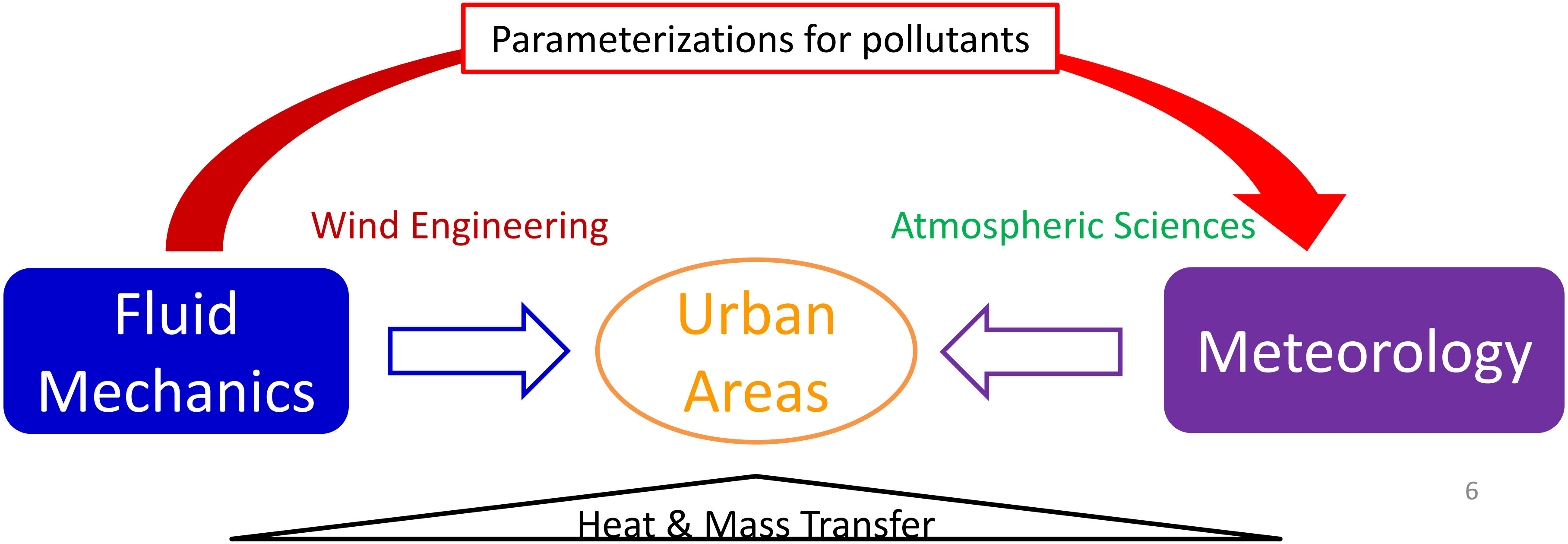
- Numerical methods
  - Finite difference
  - Finite volume
  - Finite element

- Parallelization
  - Domain decomposition



Scientific Objective

- Develop large-scale computer models simulating various atmospheric processes
- Elucidate the coupling between air pollution physics & chemistry in urban areas
- Formulate sophisticated parameterizations for chemically reactive pollutant inventory as functions of building morphology



Introduction to CFD

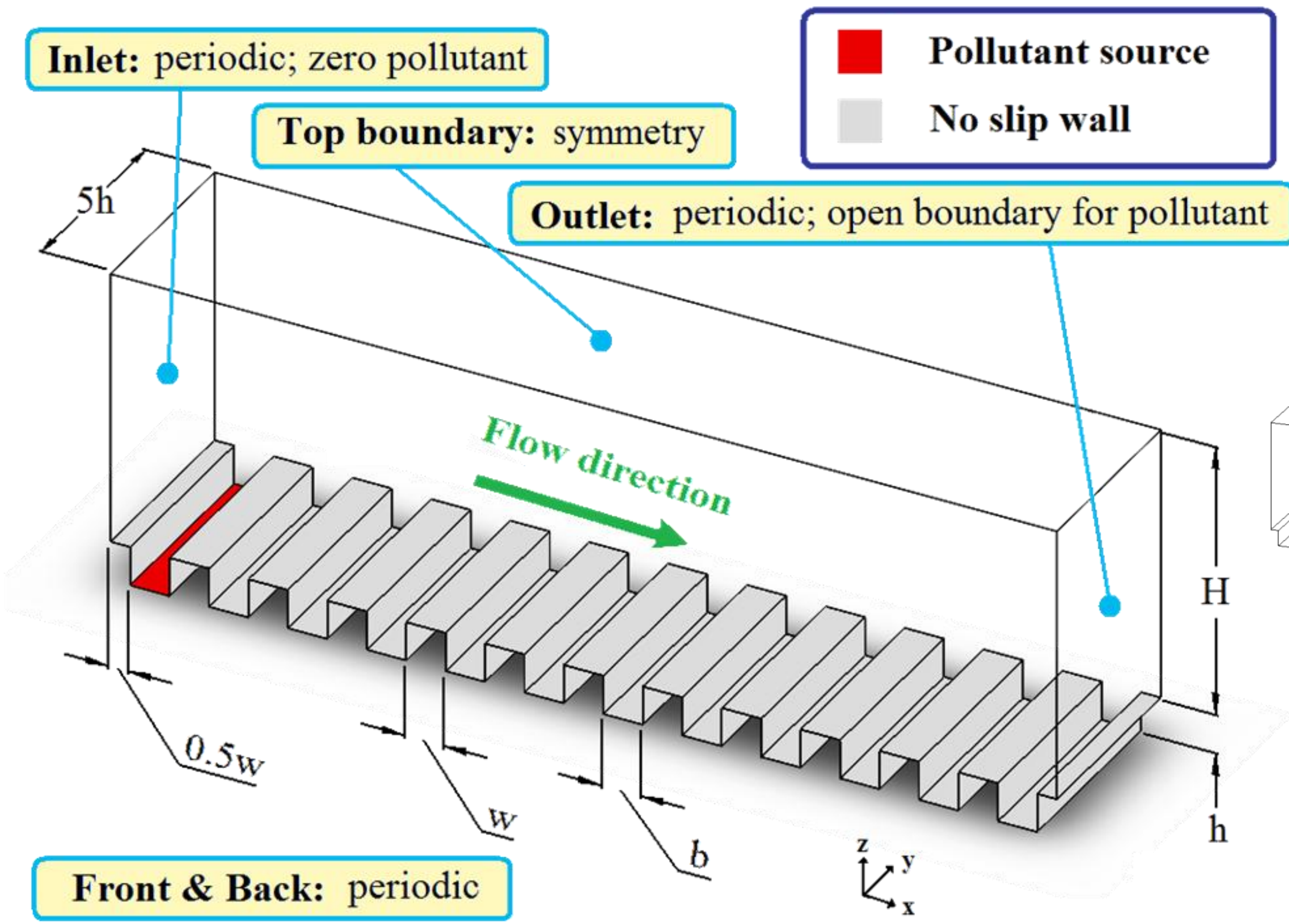
- Currently, 3 types of models are commonly used for resolving/modeling fluid turbulence.
  - *k-ε* model (RANS based)
  - Large-eddy simulation (LES)
  - Direct numerical simulation (DNS)

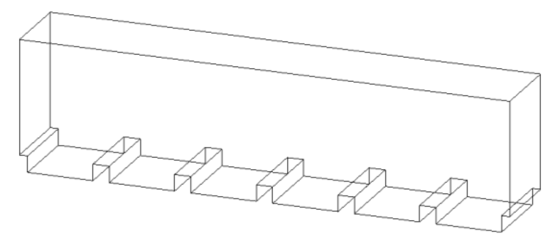
Model	*k-ε* model	**LES**	**DNS**
Accuracy	Lower		Higher
Computational cost	Relatively cheap	Expensive	Very expensive

Why LES?

- Pollutant dispersion is strongly correlated with atmospheric turbulence
  - *k*-*ε* model assumes isotropic turbulent kinetic energy (TKE) but the near-wall turbulence over 2D/3D roughness is highly anisotropic
- Study of the turbulence structure of individual components (i.e.: stream-wise fluctuation component) cannot be achieved using *k*-*ε* turbulence model.
- DNS is computationally too demanding (at the moment) for handling turbulence of large length scale.
  - e.g. atmospheric turbulence.

Computational Domain



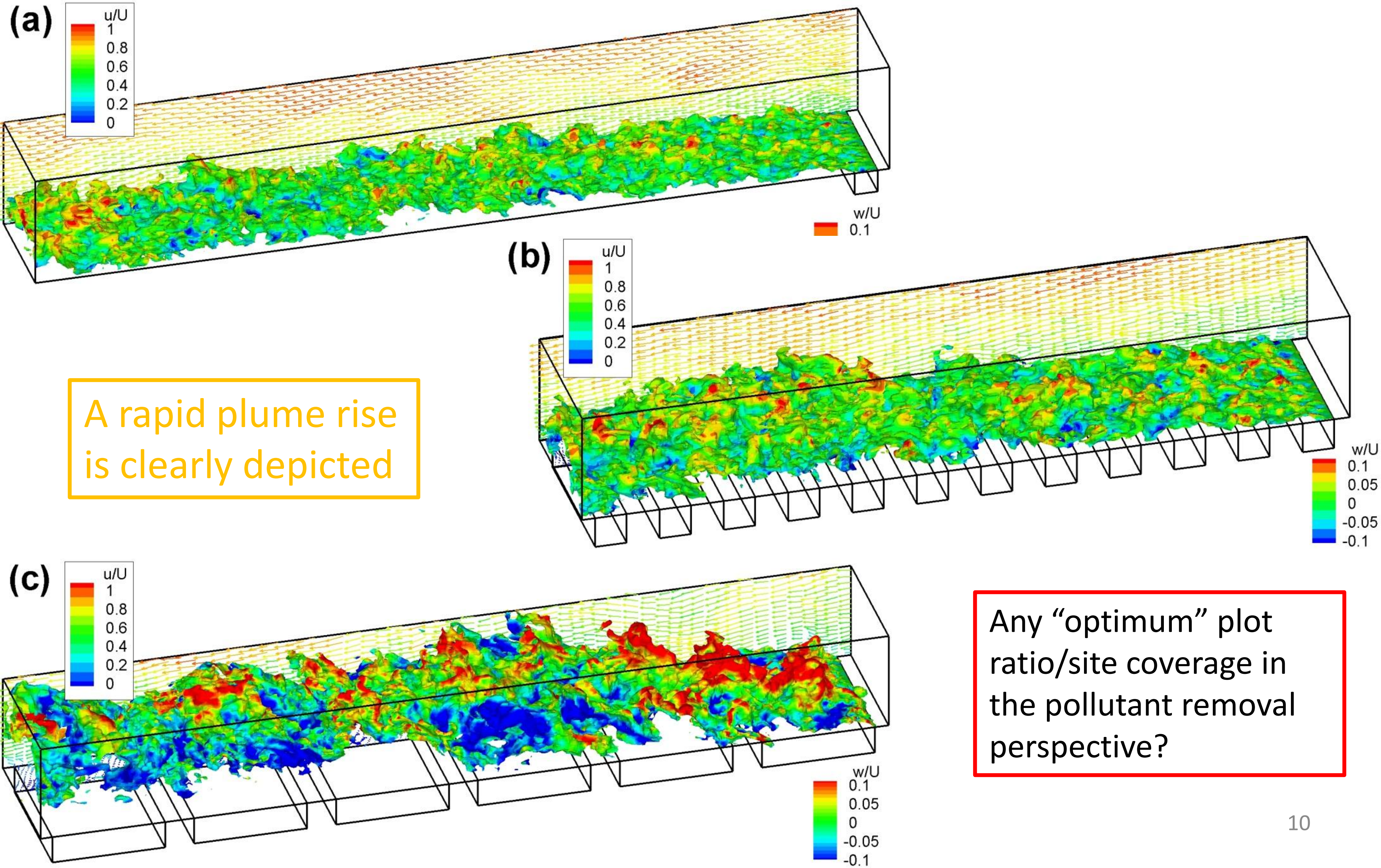


AR=0.25

AR (Aspect ratio) = h/b

AR=1.0

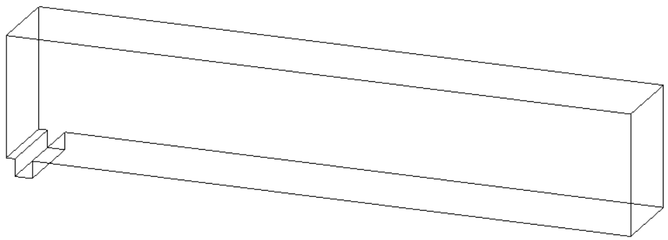
Pollutant Dispersion over Urban Fabrics



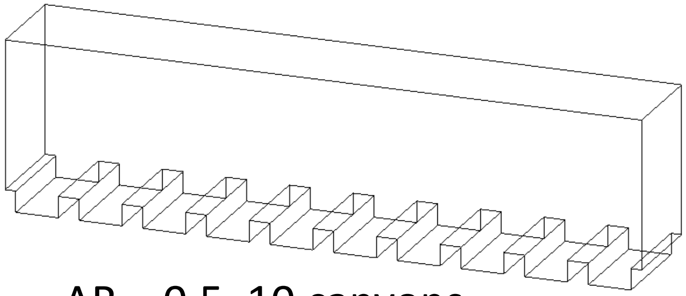
A rapid plume rise is clearly depicted

Any "optimum" plot ratio/site coverage in the pollutant removal perspective?

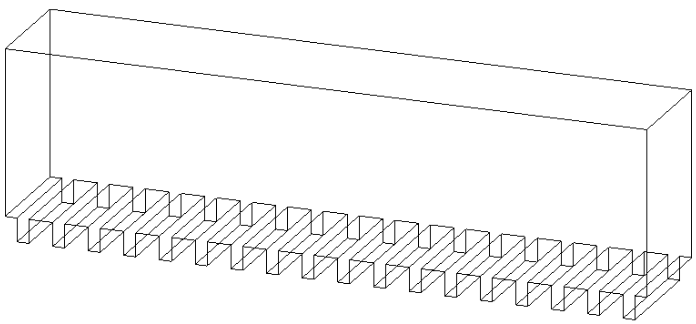
Some Other ARs



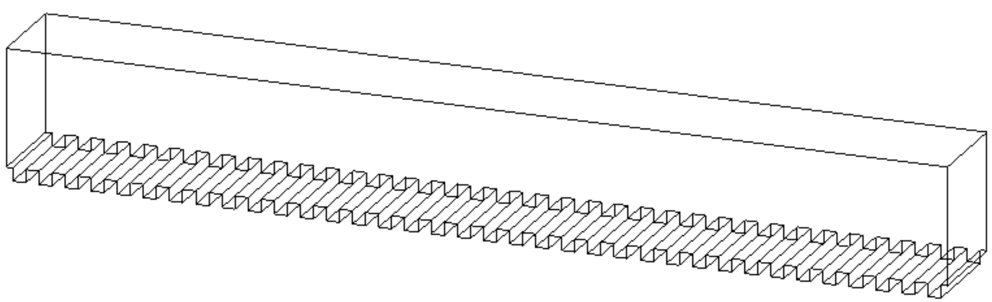
AR = 1, single canyon (control)



AR = 0.5, 10 canyons



AR = 2.0, 18 canyons

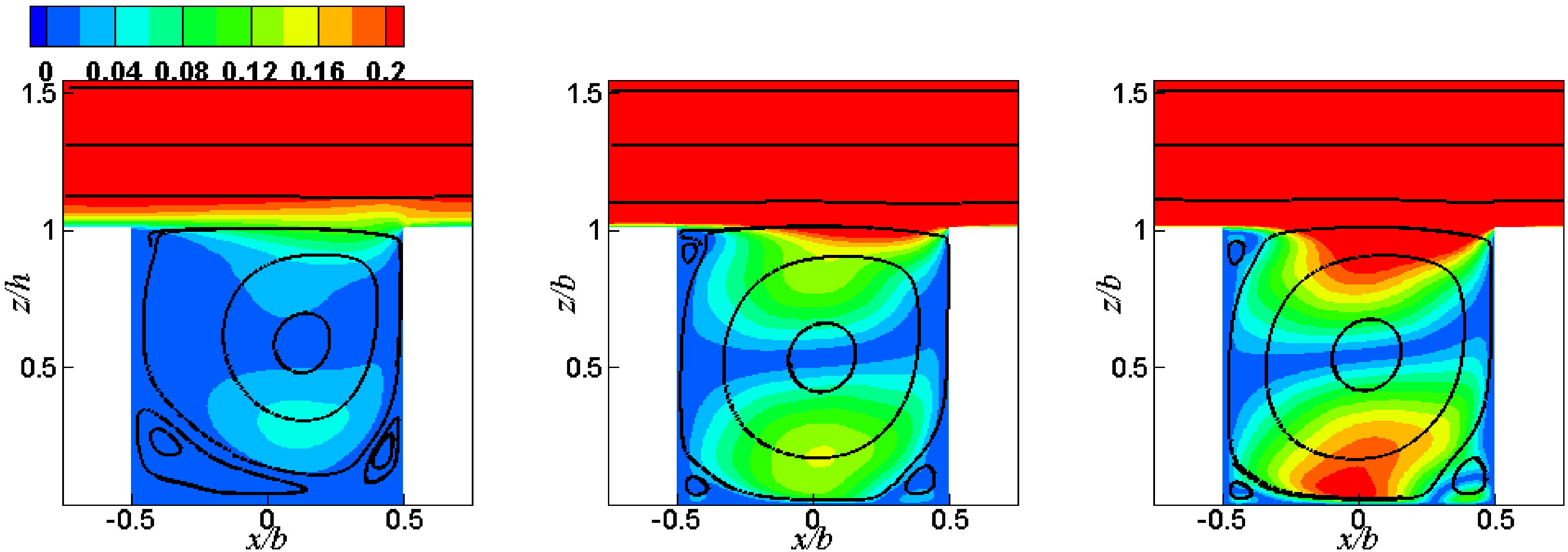


AR = 1.0, 36 canyons

Pollutant Transport in Stratification

- Contour of wind speed & streamlines

$$\mathrm{Ri} = \frac{gh}{U_0^2} \times \frac{(\Theta_0 - \Theta_w)}{\Theta_0}$$



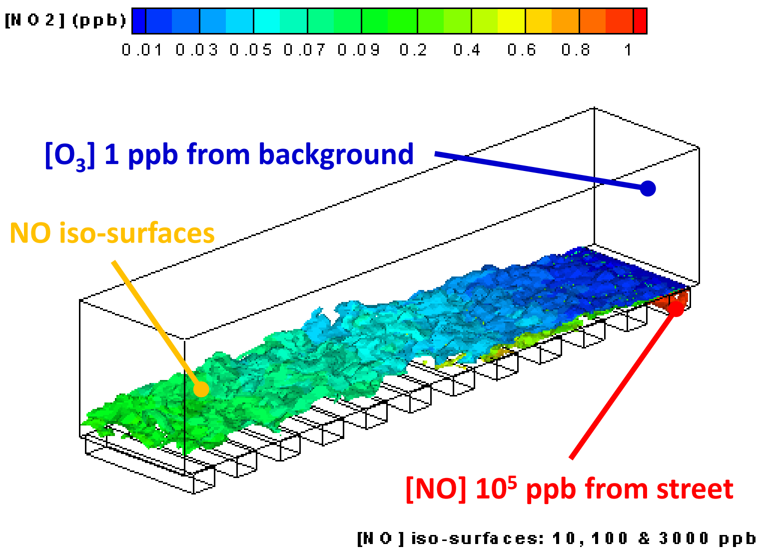
Stable stratification
Ri = 0.3

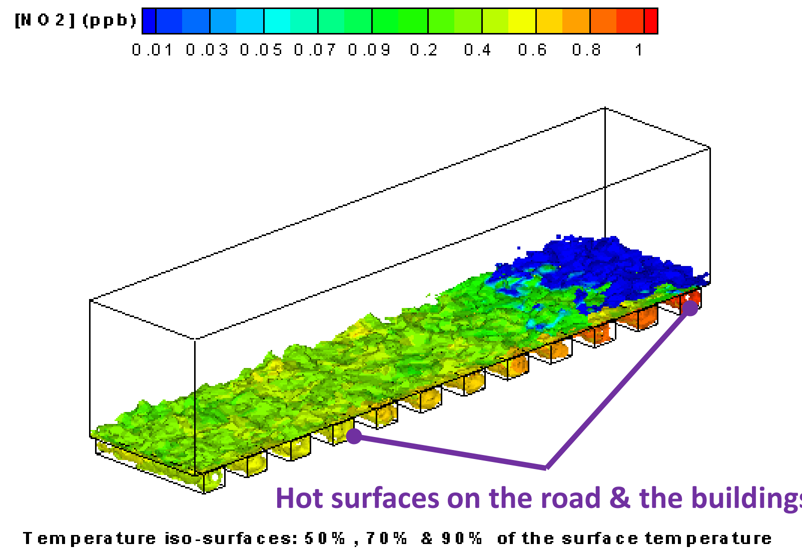
Neutral stratification
Ri = 0

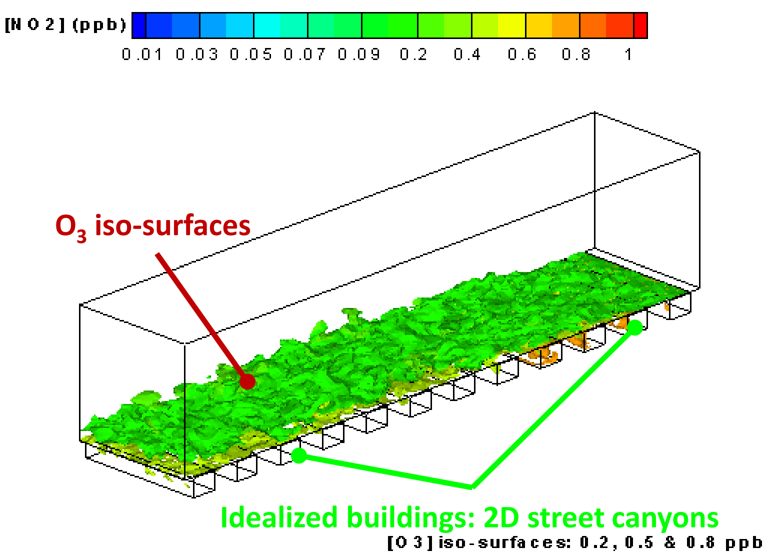
Unstable stratification
Ri = -0.25

Do we under/over estimate the pollutant removal capability of our cities in daytime/nighttime atmospheric boundary layer?

LES of Chemically Reactive Pollutants







- Simple reversible NO_x-O_3 chemistry

$$NO_2 \xrightarrow{h\nu,\, J_1} NO + O$$

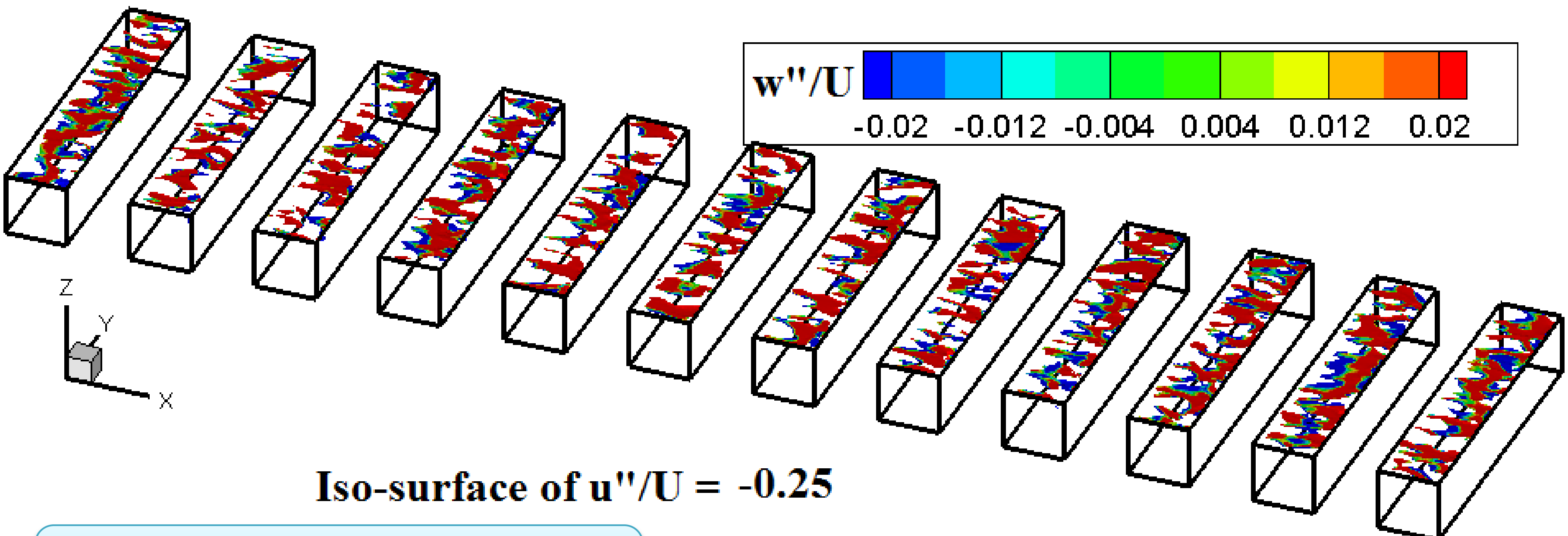
$$O + O_2 + M \xrightarrow{k_2} O_3 + M$$

$$O_3 + NO \xrightarrow{k_3} NO_2 + O_2$$

How is the non-linear coupling between air pollution physics & chemistry?

Pollutant Removal Mechanism [1/3]

Snap shot of iso-surfaces of streamwise fluctuation velocity at roof level



***u*" < 0 represents deceleration**

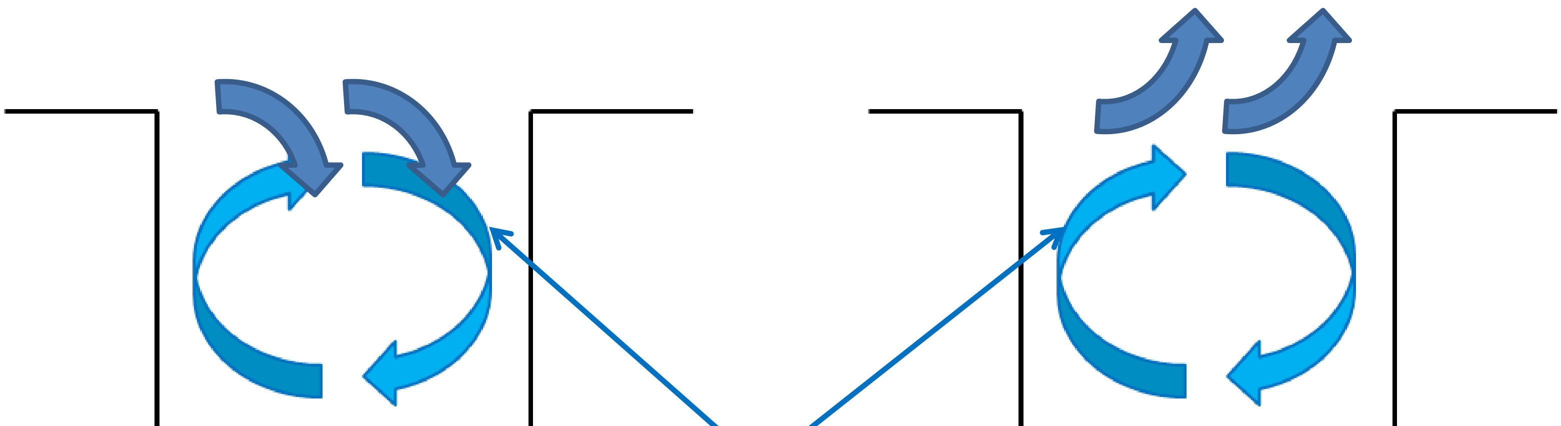
***w"* ≈ *w* at roof level**

Large amount of decelerating, up-rising air masses are located along the roof level.

Pollutant Removal mechanism [2/3]

The accelerating air masses ($u'' > 0$) carry the background pollutant into the street canyon by sweeps.

The decelerating air masses ($u'' < 0$) remove the ground-level pollutant to the UBL by ejections.



The primary re-circulation mixes the pollutant within the street canyon.

Pollutant Removal mechanism [3/3]

With pollutant sources

Pollutant removal by ejections	>>	pollutant entrainment by sweeps
	≈	

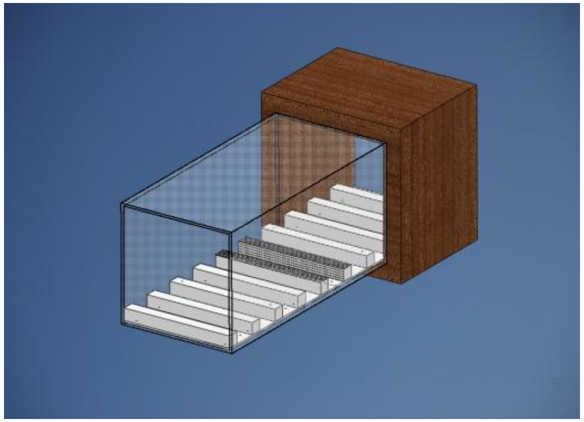
Without pollutant source

What is the role of atmospheric turbulence in pollutant removal over urban areas?

Laboratory Validation

- Wind tunnel (neutral + unstable) & water channel experiments (stable) to assess the LES results



- Other wind tunnels & water channels in HKU

Complementary solutions to the air pollutant transport over urban areas.

Future Work (in the next 2 years)

- Large-scale scientific computing
  - Increase the computation size by 1 to 2 order of magnitudes (100 to 10^3 million grid points)
  - Fundamental understanding of turbulent flow, & heat & mass transfer over urban roughness
- Use Asian cities & Hong Kong as platforms/models to examine the urban climate & pollutant transport characteristics
  - Demonstrate the feasibility of using computer models for urban climate & air quality studies
  - Applicable to other developing cities in China & the world
- Deliverables & long-term impact
  - Non-CFD models/parameterizations for other air quality applications
  - Accidental/emergency/health risk assessments